

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SUDHAKAR PATEL Examiner #: 77018 Date: 4/30/03
 Art Unit: 1624 Phone Number 308 477-9 Serial Number: 16314228 10808272
 Mail Box and Bldg/Rm Location: CMA 411 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: DERIVED MAZENIUM DILATIT, Compo. & USE THEREOF
& method of making same

Inventors (please provide full names): HRAIBI ET AL

Earliest Priority Filing Date: 7/3/1997

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Need info & comp. / compositions of use
 NO synthesis
 compounds of claim 21
 for
 open R2
 closed R1
 $R_1 - \text{CH}_2 = N(\text{R}3)R_4$ open
 closed R3
 $\text{N}_2\text{O}_2\text{E}$

Formula IV

△ Compounds of claim 22
 $\text{R}_1 - N(\text{R}3) - \text{C}(\text{R}2) - \text{R}_1$
 open R3
 closed R2
 open R5
 closed R6
 $\text{R}_1 - C - \text{N}(\text{R}3) - \text{C}(\text{R}2) - \text{R}_1$

Need & $\text{R}_1 - \text{C}(\text{R}2) - \text{R}_1$ in parent
 $\text{R}_1 - \text{C}(\text{R}2) - \text{R}_1$

POINT OF CONTACT:
 PAUL SCHULWITZ
 TECHNICAL INFO. SPECIALIST
 3M 6906 TEL. 1703) 305-1954

STAFF USE ONLY

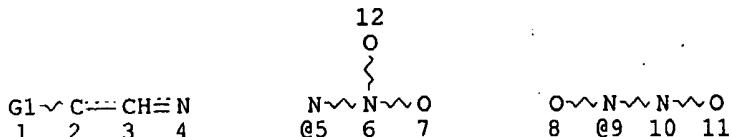
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 Searcher Location: _____
 Date Searcher Picked Up: 5/1
 Date Completed: 5/1
 Searcher Prep & Review Time: 30
 Clerical Prep Time: _____
 Online Time: 76

Type of Search

Vendors and cost where applicable

NA Sequence (#) STN 132972
 AA Sequence (#) Dialog
 Structure (#) 2.1000
 Bibliographic Dr.Link
 Litigation Lexis/Nexis
 Fulltext Sequence Systems
 Patent Family WWW/Internet
 Other Other (specify)

=> d que
L22 STR



VAR G1=5/9

NODE ATTRIBUTES:

NSPEC IS RC AT 2
NSPEC IS RC AT 4
CONNECT IS E2 RC AT 5
CONNECT IS E3 RC AT 6
CONNECT IS E1 RC AT 7
CONNECT IS E1 RC AT 8
CONNECT IS E3 RC AT 9
CONNECT IS E2 RC AT 10
CONNECT IS E1 RC AT 11
CONNECT IS E1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L24 16 SEA FILE=REGISTRY SSS FUL L22
L25 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L24

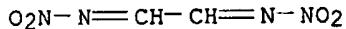
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L25 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2001:502352 HCAPLUS
DOCUMENT NUMBER: 135:256880
TITLE: DFT studies for the substituent effect on the
Diels-Alder reaction of 1,4-diaza-1,3-butadienes
AUTHOR(S): Lee, Gab-Yong
CORPORATE SOURCE: Department of Chemistry, Catholic University of Taegu,
Kyongsan, 712-702, S. Korea
SOURCE: Journal of the Korean Chemical Society (2001), 45(3),
207-212
CODEN: JKCSER; ISSN: 1017-2548
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: Korean
AB DFT calcns. have been performed on several substituted
1,4-diaza-1,3-butadienes (1,4-DABs) with electron donating and withdrawing
groups at the terminal two nitrogens to investigate the reactivity of
Diels-Alder reaction with acrolein. The calcd. FMO (frontier MO) energies
for the optimized 1,4-disubstituted-1,4-DABs have been used to explain
both normal and inverse electron demand Diels-Alder reactions. It is
shown that the electron donating and withdrawing substituents lead to the

normal (HOMO diene controlled) and inverse electron demand (LUMO diene controlled) Diels-Alder reactions, resp.

IT 362048-17-7
 RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (DFT studies for the substituent effect on the Diels-Alder reaction of 1,4-diaza-1,3-butadienes)

RN 362048-17-7 HCAPLUS
 CN Ethanediiimine, N,N'-dinitro- (9CI) (CA INDEX NAME)



L25 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 2000:540636 HCAPLUS
 DOCUMENT NUMBER: 133:281294
 TITLE: Reaction of Nitric Oxide at the .beta.-Carbon of Enamines. A New Method of Preparing Compounds Containing the Diazeniumdiolate Functional Group
 AUTHOR(S): Hrabie, Joseph A.; Arnold, Ernst V.; Citro, Michael L.; George, Clifford; Keefer, Larry K.
 CORPORATE SOURCE: Analytical Chemistry Laboratory and Intramural Research Support Program SAIC Frederick, National Cancer Institute-Frederick Cancer Research and Development Center, Frederick, MD, 21702, USA
 SOURCE: Journal of Organic Chemistry (2000), 65(18), 5745-5751
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

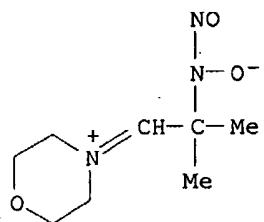
AB The reaction of nitric oxide (NO) with enamines has been investigated. Unlike previously reported reactions of NO as a free radical with alkenes, the electrophilic addn. of NO to the .beta.-carbon of enamines results in the formation of compds. contg. the diazeniumdiolate functional group (-[N(O)NO]-). This reaction between NO and enamines has been shown to be quite general and a variety of enamine-derived diazeniumdiolates have been isolated and characterized. While enamines derived from aldehydes and ketones whose structures allow for sequential multiple electrophilic addns. tended to undergo overreaction leading to unstable products, it has been shown that this complication may be overcome by suitable choice of reaction solvent. The products obtained may exist as zwitterionic iminium salts or as neutral species depending upon the structure of the parent enamine. The diazeniumdiolate derived from 1-(N-morpholino)cyclohexene is unique among the new compds. in that it spontaneously releases NO upon dissoln. in buffered aq. soln. at pH 7.4 and 37 .degree.C. While the total quantity of NO released by this material (ca. 78 of the theor. 2 mol) is apparently limited by a competing reaction in which it hydrolyzes to an .alpha.-diazeniumdiolated carbonyl compd. and the parent amine, this feature may prove to be of great value in the development of multiaction pharmaceuticals based upon this new type of NO-releasing compd. Reports of enzymic (oxidative) release of NO from previously known carbon-bound diazeniumdiolates also suggest that analogs of these compds. may be useful as pharmaceutical agents. This new method of introducing the relatively rarely studied diazeniumdiolate functional group into org. compds. should lead to further research into its chem. and biol. properties.

IT 219810-03-4P 219810-04-5P 219810-05-6P
 300398-58-7P 300398-59-8P 300398-60-1P
 300398-61-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of diazeniumdiolates from enamines and nitric oxide release
 therefrom)

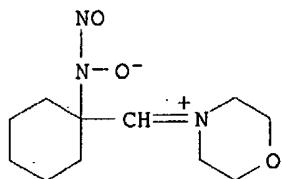
RN 219810-03-4 HCPLUS

CN Morphinium, 4-[2-(hydroxynitrosoamino)-2-methylpropylidene]-, inner salt
 (9CI) (CA INDEX NAME)



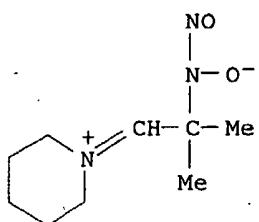
RN 219810-04-5 HCPLUS

CN Morphinium, 4-[(1-hydroxynitrosoamino)cyclohexyl]methylene-, inner
 salt (9CI) (CA INDEX NAME)



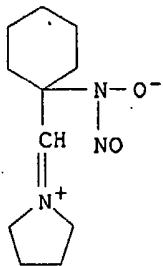
RN 219810-05-6 HCPLUS

CN Piperidinium, 1-[2-(hydroxynitrosoamino)-2-methylpropylidene]-, inner salt
 (9CI) (CA INDEX NAME)

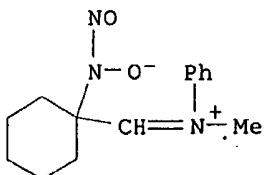


RN 300398-58-7 HCPLUS

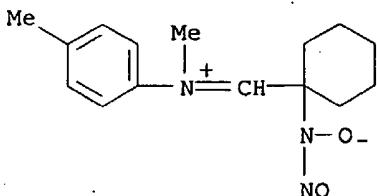
CN Pyrrolidinium, 1-[(1-hydroxynitrosoamino)cyclohexyl]methylene-, inner
 salt (9CI) (CA INDEX NAME)



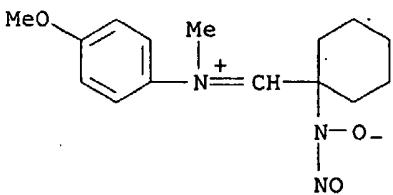
RN 300398-59-8 HCPLUS

CN Benzenaminium, N-[(1-(hydroxynitrosoamino)cyclohexyl)methylene]-N-methyl-,
inner salt (9CI) (CA INDEX NAME)

RN 300398-60-1 HCPLUS

CN Benzenaminium, N-[(1-(hydroxynitrosoamino)cyclohexyl)methylene]-N,4-
dimethyl-, inner salt (9CI) (CA INDEX NAME)

RN 300398-61-2 HCPLUS

CN Benzenaminium, N-[(1-(hydroxynitrosoamino)cyclohexyl)methylene]-4-methoxy-
N-methyl-, inner salt (9CI) (CA INDEX NAME)

REFERENCE COUNT:

58

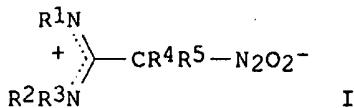
THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

May 1, 2003

L25 ANSWER 3 OF 6 HCPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1999:48699 HCPLUS
 DOCUMENT NUMBER: 130:125081
 TITLE: Preparation of novel nitric oxide-releasing amidine-
 and enamine-derived diazeniumdiolates as drugs
 INVENTOR(S): Hrabie, Joseph A.; Keefer, Larry K.
 PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
 SOURCE: PCT Int. Appl., 59 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9901427	A2	19990114	WO 1998-US13723	19980701
WO 9901427	A3	19990325		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HR, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9882815	A1	19990125	AU 1998-82815	19980701
AU 726861	B2	20001123		
EP 1000023	A2	20000517	EP 1998-933062	19980701
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002510320	T2	20020402	JP 1999-507350	19980701
US 6232336	B1	20010515	US 2000-446653	20000330
US 2001025052	A1	20010927	US 2001-825073	20010403
US 6511991	B2	20030128		
PRIORITY APPLN. INFO.:			US 1997-51690P	P 19970703
			WO 1998-US13723	W 19980701
			US 2000-446653	A3 20000330

OTHER SOURCE(S): MARPAT 130:125081
 GI



AB Amidine- and enamine-derived diazeniumdiolates selected from I,
 $\text{R}^2\text{R}^3\text{N}(\text{R}^1\text{NH})\text{C}:\text{CR}^4(\text{N}_2\text{O}_2^-)$, $\text{R}^2\text{R}^3\text{N}(\text{R}^1\text{NH})\text{C}:\text{C}(\text{N}_2\text{O}_2^-)\text{--}^2$ [$\text{R}^1\text{--R}^3 = \text{H}$,
 (un)substituted C1-12 alkyl, (un)substituted C3-8 cycloalkyl, N- or
 O-contg. C3-8 heterocycl, (un)substituted (tetrahydro)naphthyl, etc.;
 $\text{R}^4, \text{R}^5 = \text{H}$, (un)substituted C1-12 alkyl, (un)substituted Ph,
 (un)substituted piperazino, morpholino, etc.; R1R2N, R2R3N can form
 (un)substituted C3-8 heterocycl; R4R5C can form (un)substituted C3-8
 cycloalkyl; etc.] and related compds., useful for treatment of biol.

disorders treatable with NO, were prep'd. A method of prep'g. the title diazeniumdiolates by treating primary or secondary amines with acetamidating agents and treating the resulting acetamidines with NO(g) is also claimed. For example, a soln. of 1.00 g idazoxan-HCl in a mixt. of 0.95 mL 25% NaOMe in MeOH and 3 mL MeOH was dild. with 40 mL MeCN, the ppt. (NaCl) was removed by filtration and the soln. was treated with NO for 21 h to give 0.62 g idazoxan-bis(nitric oxide) adduct m. 152-154.degree.. The latter showed initial NO release of 5.25 .times. 10-11 mole NO/min/mg which gradually increased to 1.41 .times. 10 -10 mole/NO/mg after 4 days and then decreased, reaching 0 by day 16.

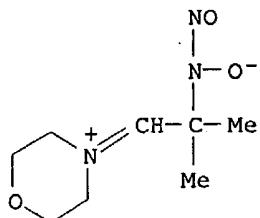
IT 219810-03-4P 219810-04-5P 219810-05-6P
219810-06-7P 219810-07-8P 219810-08-9P

219810-09-OP

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prep'n. of novel nitric oxide-releasing amidine- and enamine-derived diazeniumdiolates as drugs)

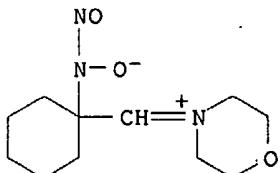
RN 219810-03-4 HCPLUS

CN Morpholinium, 4-[2-(hydroxynitrosoamino)-2-methylpropylidene]-, inner salt (9CI) (CA INDEX NAME)



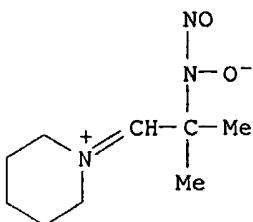
RN 219810-04-5 HCPLUS

CN Morpholinium, 4-[[1-(hydroxynitrosoamino)cyclohexyl]methylene]-, inner salt (9CI) (CA INDEX NAME)

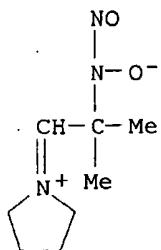


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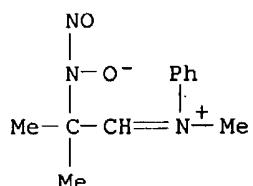
CN Piperidinium, 1-[2-(hydroxynitrosoamino)-2-methylpropylidene]-, inner salt (9CI) (CA INDEX NAME)



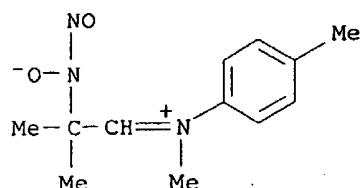
RN 219810-06-7 HCPLUS
 CN Pyrrolidinium, 1-[2-(hydroxynitrosoamino)-2-methylpropylidene]-, inner salt (9CI) (CA INDEX NAME)



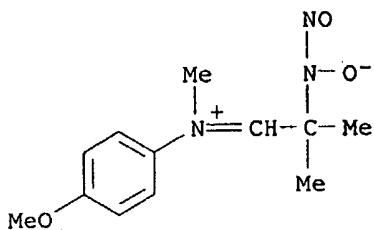
RN 219810-07-8 HCPLUS
 CN Benzenaminium, N-[2-(hydroxynitrosoamino)-2-methylpropylidene]-N-methyl-, inner salt (9CI) (CA INDEX NAME)



RN 219810-08-9 HCPLUS
 CN Benzenaminium, N-[2-(hydroxynitrosoamino)-2-methylpropylidene]-N,4-dimethyl-, inner salt (9CI) (CA INDEX NAME)



RN 219810-09-0 HCPLUS
 CN Benzenaminium, N-[2-(hydroxynitrosoamino)-2-methylpropylidene]-4-methoxy-N-methyl-, inner salt (9CI) (CA INDEX NAME)



1.25 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1992:650902 HCAPLUS

ACCESSION NUMBER: 1999-0001
DOCUMENT NUMBER: 117:250902

DOCUMENT NUMBER: 117.20092
TITLE: Ab initio molecular orbital study of nitrogen-containing polyenes with donor-acceptor substituents: dipole moment and static first hyperpolarizability

AUTHOR(S): Tsunekawa, Tetsuya; Yamauchi, Kizashi

CORPORATE SOURCE: Polym. Res. Lab., Toray Ind., Inc., Shiga, 520, Japan

SOURCE: Journal of Physical Chemistry (1992), 96(25), 10268-75

SOURCE: JOURNAL OF PHYSICAL CHEMISTRY, VOL. 68, NO. 10, OCTOBER 1964
CODEN: JPCHAX; ISSN: 0022-3654

DOCUMENT TYPE: CODEN: SICHAU; ISSN: 0022-0833
Journal

DOCUMENT TYPE: Journal
LANGUAGE: English

LANGUAGE: English
AB Ab initio coupled-perturbed

AB Ab initio coupled-perturbed Hartree-Fock (CPHF) calcns. have been carried out to clarify the relation between dipole moment (.mu.) and first hyperpolarizability (.beta.) of nitrogen-contg. .pi.-conjugated polyenes with donor and acceptor substituents attached on the end. Systematic calcns. on the polyene-like model compds. indicate that nitrogen-atom substitutions in .pi.-conjugated systems fluctuate .mu. values and gradually decrease .beta. values with increasing no. of N atoms. From the calcd. results, several tendencies are recognized for the changes of .mu. and .beta. induced by the N substitution. The mols. with N at an even-numbered position counted from an electron-accepting nitro group have larger .beta. but smaller .mu. than those with N at an odd-numbered position, which is the other position of the same double bond. Esp., introduction of a single N into the even-numbered position of hexatriene analogs decreases the .mu. value as controlling the redn. of .beta. value. These ab initio results support previous conclusions based on semiempirical CNDO/S calcns. of stilbene and benzylideneaniline mols. The analyses of MOs and full SCI calcns. of the electronic transitions for the model compds. have revealed the intrinsic effects of N substitutions; the decrease of .beta. is mainly attributed to the blue shift of the absorption max., and the N substitution at the even-numbered position counted from nitro group enhances the induced polarization through the effective variations of the energy levels and shapes of the frontier .pi. orbitals. N substitutions at specific positions provide an effective approach in designing mols. with relatively small .mu. but large .beta., which are desirable from the viewpoint of crystal engineering of nonlinear optical materials.

IT 144565-55-9

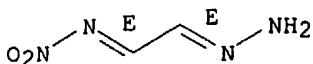
RL: PRP (Properties)

(dipole moment and hyperpolarizability of, ab initio calcn. of)

RN 144565-55-9 HCAPLUS

CN Acetaldehyde, (nitroimino)-, hydrazone, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L25 ANSWER 5 OF 6 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1992:213749 HCPLUS

DOCUMENT NUMBER: 116:213749

TITLE: Ab initio CPHF calculations of first hyperpolarizabilities of nitrogen-containing polyenes with donor-acceptor substituents

AUTHOR(S): Tsunekawa, Tetsuya; Yamaguchi, Kizashi

CORPORATE SOURCE: Polym. Res. Lab., Toray Ind. Inc., Otsu, 520, Japan

SOURCE: Chemical Physics Letters (1992), 190(6), 533-8

CODEN: CHPLBC; ISSN: 0009-2614

DOCUMENT TYPE: Journal

LANGUAGE: English

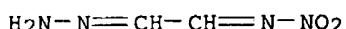
AB Ab initio CPHF calcns. of static hyperpolarizabilities (β) were carried out in order to clarify the effects of nitrogen-atom substitution in π -conjugated chains with donor-acceptor substituents. The β values decrease gradually with the no. of nitrogen atoms, and change drastically with the position of nitrogen-atom substitution in the polyenes. The effects of nitrogen-atom substitution are explained by the energy levels and the shapes of the frontier orbitals.

IT 141122-75-0

RL: PRP (Properties)
(first hyperpolarizability of, calcd. by coupled-perturbed Hartree-Fock, HOMO-LUMO energy gap in relation to)

RN 141122-75-0 HCPLUS

CN Acetaldehyde, (nitroimino)-, hydrazone (9CI) (CA INDEX NAME)



L25 ANSWER 6 OF 6 HCPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1976:559592 HCPLUS

DOCUMENT NUMBER: 85:159592

TITLE: Preparation and properties of N-nitroso-.alpha.-hydroxylamino oximes

AUTHOR(S): Volodarskii, L. B.; Tormysheva, N. Yu.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, USSR

SOURCE: Izvestiya Sibirskogo Otdeleniya Akademii Nauk SSSR,

Seriya Khimicheskikh Nauk (1976), (4), 136-40

CODEN: IZSKAB; ISSN: 0002-3426

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Treatment of $\text{RC}(\text{:NOH})\text{CMe}_2\text{NOH}$ ($\text{R} = \text{Ph}, \text{Me}, \text{H}$) with amyl nitrite gave

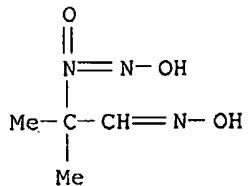
$\text{RC}(\text{:NOH})\text{CMe}_2\text{N}(\text{OH})\text{NO}$ (I), which when treated with EtONa gave

$\text{RC}(\text{:NOH})\text{CMe}_2\text{N}(\text{O}): \text{NONa}$. Acetylation of I ($\text{R} = \text{Ph}$) gave

$\text{PhC}(\text{:NOAc})\text{CMe}_2\text{N}(\text{OH})\text{NO}$, which gave the p-toluenesulfonate deriv. Treatment of I ($\text{R} = \text{Me}$) with Me_2SO_4 gave $\text{MeC}(\text{:NOH})\text{CMe}_2\text{N}(\text{NO})\text{OMe}$.

May 1, 2003

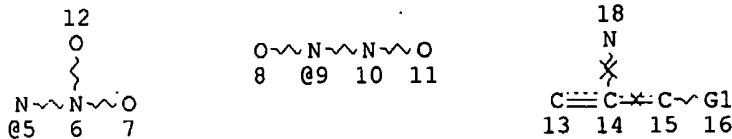
IT 60983-74-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 60983-74-6 HCAPLUS
CN Propanal, 2-(hydroxy-NNO-azoxy)-2-methyl-, oxime, monosodium salt (9CI)
(CA INDEX NAME)



● Na

=> d que

L29 STR



VAR G1=5/9

NODE ATTRIBUTES:

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NSPEC IS RC AT 13
CONNECT IS E2 RC AT 5
CONNECT IS E3 RC AT 6
CONNECT IS E1 RC AT 7
CONNECT IS E1 RC AT 8
CONNECT IS E3 RC AT 9
CONNECT IS E2 RC AT 10
CONNECT IS E1 RC AT 11
CONNECT IS E1 RC AT 12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
  
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GRAPH ATTRIBUTES:

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13
  
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STEREO ATTRIBUTES: NONE

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L31 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L30
  
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=> d ibib abs hitstr l31 1-3

L31 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1999:454861 HCAPLUS

DOCUMENT NUMBER: 131:257160

TITLE: Azetidine and its mono-, di-, and trinitro-substituted derivatives. Computer modeling of decomposition reactions

AUTHOR(S): Porollo, Aleksei A.; Petukhova, Tatyana V.; Ivshin, Victor P.; Pivina, Tatyana S.; Lushnikov, Dmitrii E.

CORPORATE SOURCE: Mari State Univ., Yoshkar-Ola, 424000, Russia

SOURCE: International Annual Conference of ICT (1999), 30th, 15/1-15/13

CODEN: IACIEQ; ISSN: 0722-4087

PUBLISHER: Fraunhofer-Institut fuer Chemische Technologie

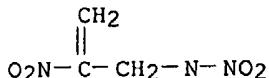
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The modeling of thermal decompn. of azetidine and its mono,- di,- and trinitro-substitute derivs. on the basis of recombination reaction networks (RRN) was investigated. Generation of intermediate particles was carried out using heuristic rules, developed after generalization of exptl. data on decompn. mechanisms for major classes of energetic compds. For each target compd. program generates comprehensive set of hypothetical mechanisms of thermal decompn. In the case of azetidine there is a wide

fraction of alkyls and alkyl amines in products resulting by the lack of O in mol of source substance.. NO₂ groups increase the probability of predominance of X-NO₂ bond dissociation as initial stage of thermolysis beside the homolysis of C-C or C-N bonds in azetidine rings.

IT 149050-12-4
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
 (heat of formation of thermolysis products of azetidine and its mono-, di-, and trinitro-substituted derivs.)
 RN 149050-12-4 HCPLUS
 CN Amidogen, nitro(2-nitro-2-propenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

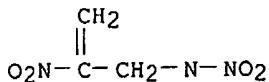
L31 ANSWER 2 OF 3 HCPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1998:408236 HCPLUS
 DOCUMENT NUMBER: 129:148691
 TITLE: Gas-Phase Pyrolysis of 1,3,3-Trinitroazetidine: Shock Tube Kinetics
 AUTHOR(S): Zhang, Yi-Xue; Bauer, S. H.
 CORPORATE SOURCE: Chemistry Department, Baker Chemical Laboratory, Cornell University, Ithaca, NY, 14853, USA
 SOURCE: Journal of Physical Chemistry A (1998), 102(29), 5846-5856
 CODEN: JPCAFH; ISSN: 1089-5639
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Vapors of 1,3,3-trinitroazetidine (TNAZ) were pyrolyzed in a single-pulse shock tube, under high diln. in Ar, over the temp. range 750-1100 K (reflected shocks). The decay of TNAZ and the appearance of the reactive intermediate, NO₂, were followed spectrophotometrically at 271 and 405 nm, resp., in real time via a multiple-pass quartz extension of the shock tube terminus. Samples of the major products that were generated during 1.5 ms residence time and wave quenched were identified and quantitated by GC and FTIR. The unimol. rate const. (high-pressure limit) for dissociation of TNAZ under our exptl. conditions is k_{uni} = 1013.96.+-0.63 exp{(-19900 .+-. 1190)/T}, s⁻¹. Successive fissions of NO₂ groups were indicated by the time-dependent absorption levels at 405 nm. A gas-phase FTIR spectrum of TNAZ recorded at .apprx.110.degree. provided the missing data for computing the thermochem. parameters for this compd. Then the partition of its decompn. products (minimal free energy) could be calcd. for 900 and 1100 K. The obsd. product distributions differ markedly from those calcd., indicating that the overall reaction is kinetically limited. Several possible reaction pathways at the early stages of the pyrolysis are discussed, and a preliminary reaction mechanism consisting of 46 chem. reactions is proposed. Simulations based on this mechanism agree reasonably well with the exptl. results despite uncertainties. Addnl. work on the pyrolyses of mono- and dinitro substituted azetidines is

May 1, 2003

needed to det. the relative importance of the various dissociation pathways in the present system.

IT 149050-12-4
 RL: FMU (Formation, unclassified); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
 (reactive intermediate; pyrolysis of 1,3,3-trinitroazetidine (TNAZ) in single-pulse shock tube)
 RN 149050-12-4 HCAPLUS
 CN Amidogen, nitro(2-nitro-2-propenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2003 ACS
 ACCESSION NUMBER: 1993:494726 HCAPLUS
 DOCUMENT NUMBER: 119:94726
 TITLE: Energy changes associated with some decomposition steps of 1,3,3-trinitroazetidine. A non-local density functional study
 AUTHOR(S): Politzer, Peter; Seminario, Jorge M.
 CORPORATE SOURCE: Department of Chemistry, University of New Orleans,
 New Orleans, LA, 70148, USA
 SOURCE: Chemical Physics Letters (1993), 207(1), 27-30
 CODEN: CHPLBC; ISSN: 0009-2614
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A non-local d. functional approach has been used to compute the energy changes for the individual steps in three proposed decompr.. pathways of 1,3,3-trinitroazetidine. The loss of the second NO₂ is the first step at which their energetics are qual. different. It is concluded that products will be obtained from all three pathways.
 IT 149050-12-4
 RL: PRP (Properties)
 (optimized geometry of)
 RN 149050-12-4 HCAPLUS
 CN Amidogen, nitro(2-nitro-2-propenyl)- (9CI) (CA INDEX NAME)

